TT 46: Poster Session: Frustrated Magnets, Quantum Magnets, Charge Order and Complex Oxides

Time: Wednesday 15:00–19:00 Location: P2/2OG

TT 46.1 Wed 15:00 P2/2OG

Manipulation of charge density waves in transition metal dichalcogenides by strain and adsorbates — •F. Cossu[1], I. Di Marco[1], and A. Akbari[1,2] — [1]Asia Pacific Center for Theoretical Physics, POSTECH, Pohang, Korea — [2]Max Planck POSTECH Center for Complex Phase Materials, POSTECH, Pohang, Korea

Interest in transition metal dichalcogenides (materials consisting of van der Waals bonded layers) has been revived due to relatively recent access to synthesis of few layers, where their characteristic structure may result in massive symmetry breaking, which lead to exotic properties in the electronic structure. Collective phases such as superconductivity and charge density waves (CDW), which may be conventional in the bulk, could in principle become unconventional in single layers. Therefore, understanding the mechanisms of emergence of these electronic phases and how they change upon external fields or doping is of great interest. Since the symmetry of the CDW induces the symmetry of the superconducting gap, it is interesting to investigate instances of symmetry change. In $NbSe_2$, charge density waves are incommensurate and follow a triangular modulation 3×3, in the bulk and in single layers. However, zones where the modulation has a stripe character have been observed in single layers. By means of ab-initio calculations, we investigate the possible scenarios beneath the occurrence of the stripe phase. In addition, adsorption by transition metals induces a hierarchy change and a reduction of the symmetry in CDW; it may be argued that, due to the nature of the adsorbate, spin-orbit effect may dominate the nature of the collective excitations.

TT 46.2 Wed 15:00 P2/2OG

Influence of inhomogeneous orderings on charge transport in a Falicov-Kimball heterostructure — •Rudolf Smorka, Martin Žonda, and Michael Thoss — Albert-Ludwigs-Universität Freiburg i. Br., Deutschland

The spinless Falicov-Kimball model outside the particle-hole symmetric point exhibits different stable inhomogeneous charge orderings. Among these are well-known charge stripes and a variety of orderings with phase separated domains, which influence the charge transport through the correlated electron system significantly. In this work, we will show these effects by investigating a heterostructure, where the Falicov-Kimball model on a finite two-dimensional lattice is located between two non-interacting semi-infinite leads. We use a combination of nonequilibrium Green's functions techniques with a sign-problem-free Monte Carlo method for finite temperatures, and simulated annealing technique for the ground state, to address steady-state transport through the system. Our study shows that different ground-state phases of the central system can lead to simple metallic-like or insulating charge transport characteristics, but also to more complicated current-voltage dependencies reflecting a multi-band character of the transmission function. As temperature is increased, there is a tendency towards formation of transient phases before the system reaches a disordered phase. This leads to nontrivial temperature dependencies of transmission function and charge current.

TT 46.3 Wed 15:00 P2/2OG

Microscopic Dynamics during Charge-Glass Formation in θ-(BEDT-TTF)$_2$TlZn(SCN)$_4$ — •Tim Thyzel[1], Tatjana Thomas[1], Kenichiro Hashimoto[2], Takahiko Sasaki[2], and Jens Müller[1] — [1]Institute of Physics, Goethe-University Frankfurt, Frankfurt (Main), Germany — [2]Institute for Materials Research, Tohoku University, Sendai, Japan

Organic charge-transfer salts allow for a systematic examination of strong electron-electron correlation in reduced dimensions. The θ-$(ET)_2X$ salts, which consist of alternating layers of conducting organic molecules $(ET)_2$ and insulating anions X, exhibit charge ordering in the conducting layers below a characteristic temperature. However, the phase transition of the electronic system to this ordered state can be avoided by rapid cooling [1]. Then, a glass-like state emerges due to the geometric frustration of the conducting lattice, which acts against the formation of long-range order. We study the system θ-$(ET)_2$TlZn$(SCN)_4$, whose lattice is more anisotropic, and thus less frustrated, than that of other θ-phase compounds. Therefore, rather high cooling rates of at least 50 K/min are required to force a transition to the charge-glass state [2]. We achieve these cooling rates using a voltage pulse method recently shown [3] to be capable of rates in excess of 1000 K/min. Resistance fluctuation spectroscopy is then employed to gain insights into the deceleration of microscopic dynamics at the liquid-glass transition [4].

[1] Adv. Mater. 29, 1601979
[2] Science 357, 1381-1385
[3] Phys. Rev. B 90, 195150
[4] Crystals 8, 166

TT 46.4 Wed 15:00 P2/2OG

Strain-induced metal-to-insulator transitions in spinel oxide thin films — •Tim Schweizer[1,2], Ulrike Niemann[1,2], Dennis Huang[1], and Hidenori Takagi[1,2,3] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Institute for Functional Matter and Quantum Technologies, University of Stuttgart, Germany — [3]Department of Physics, University of Tokyo, Japan

Spinel compounds with underlying pyrochlore lattice are known playgrounds for geometric frustration. In particular, LiV_2O_4 has attracted considerable attention due to its unconventional heavy fermion phase, which emerges at low temperatures in the absence of localized f electrons [1]. Recent studies have shown that metallic LiV_2O_4 can be driven into an insulating, charge-ordered state by applying epitaxial strain in the thin-film limit. Such an observation hints at the role of charge frustration and quantum criticality in the heavy fermion phase of LiV_2O_4. Using pulsed laser deposition, we studied thin films of LiV_2O_4 (strained and unstrained), and compared them with thin films of the distorted spinel AlV_2O_4, where a charge-ordered state was previously reported in powder samples [2].

[1] C. Urano et al., Phys. Rev. Lett. 85, 1052 (2000)
[2] K. Matsuno et al., JPS Journal, 70, 1456-1459 (2001)

TT 46.5 Wed 15:00 P2/2OG

Emergence and stability of spin-valley entangled quantum liquids in Moiré heterostructures — •Dominik Kiese, Finn Lasse Buessen, Ciaran Hickey, Simon Trebst, and Michael M. Scherer — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

Moiré heterostructures with nearly flat bands have recently been established as a new playground for strongly-correlated electron physics. The precise nature of the correlated states is yet to be understood through the application of quantum many-body methods. Essential traits of phenomenological models for Moiré heterostructures include a hexagonal superlattice, a two-valley structure, as well as extended Hubbard and Hund's interaction terms. Taking a strong-coupling perspective, these features result in generalized Heisenberg models with separate spin and valley degrees of freedom. Here, the combination of geometric frustration and enhanced quantum fluctuations may inhibit the formation of conventional magnetic order. We study such extended spin-valley Heisenberg models using functional RG methods and find rich phase diagrams exhibiting stable realms of quantum spin-valley liquid behavior. We further show that even for purely antiferromagnetic couplings, ferromagnetic order may emerge in an extensive parameter regime. We discuss the relevance of our results for trilayer graphene on hexagonal boron nitride and twisted double bilayer graphene.

TT 46.6 Wed 15:00 P2/2OG

Lifshitz Transitions in Neutral Fermi Surfaces — •Vaishnavi Jayakumar and Ciaran Hickey — Institute for Theoretical Physics, University of Cologne, 50937 Cologne, Germany

In his seminal 1960 paper, I. M. Lifshitz predicted the existence of a transition where the Fermi surface of a metal changes its topology, as a Van Hove singularity crosses the Fermi energy. These "Electronic Topological Transitions", or "Lifshitz transitions" , leave a strong imprint on thermodynamic and transport observables, and have since been observed in a variety of metals.

Here, we examine the consequences of a Lifshitz transition in a neutral Fermi surface, i.e. a metal of fermionic quasiparticles that are charge neutral. Such an exotic Fermi surface can arise in strongly correlated systems, with a paradigmatic example being the spinon Fermi

surface of a U(1) quantum spin liquid.

We discuss the unique signatures of Lifshitz transitions in neutral metals, and compare and contrast them with the conventional electronic case. Similarly, we also discuss the recently classified multicritical Lifshitz transitions and their potential experimental fingerprints in spinon Fermi surface states.

TT 46.7 Wed 15:00 P2/2OG

Quasi-molecular electronic structure of the spin-liquid candidate $Ba_3InIr_2O_9$ revealed by RIXS — Alessandro Revelli[1], •Marco Magnaterra[1], Marco Moretti Sala[2], Giulio Monaco[3], Jan Attig[4], Alexander Tsirlin[5], Tusharkanti Dey[1,5], Philipp Gegenwart[5], Tobias Fröhlich[1], Petra Becker[6], Maria Hermanns[7], Paul H. M. van Loosdrecht[1], Daniel I. Khomskii[1], Jeroen van den Brink[8], and Markus Grüninger[1] — [1]II. Physikalisches Inst., Universität zu Köln — [2]Dip. di Fisica, Politecnico di Milano, Italy — [3]Dip. di Fisica, Università di Trento, Italy — [4]Inst. fur Theoretische Physik, Universität zu Köln — [5]Experimental Physics VI, University of Augsburg — [6]Abt. Kristallographie, Inst. fur Geologie und Mineralogie, Universitat zu Köln — [7]Dep. of Physics, Stockholm University, Sweden — [8]Inst. for Theoretical Solid State Physics, IFW Dresden

We address the electronic structure of the mixed-valent iridate $Ba_3InIr_2O_9$ by means of resonant inelastic x-ray scattering (RIXS). Previously, it has been discussed as a promising candidate for quantum spin-liquid behavior [1]. It exhibits $Ir^{4.5+}$ ions in face-sharing IrO_6 octahedra forming Ir_2O_9 dimers. RIXS unravels a rich excitation spectrum below about 1.5eV. The observation of a pronounced sinusoidal RIXS interference pattern unambiguously demonstrates the quasi-molecular orbital character of the electronic states. Three t_{2g} holes are delocalized over a dimer, establishing $Ba_3InIr_2O_9$ as a cluster Mott insulator with a quasi-molecular j_{dim}=1/2 ground state.

[1] Dey et al., PRB 96, 174411 (2017).

TT 46.8 Wed 15:00 P2/2OG

Investigation of the thermodynamic effects of electron-nucleus interactions in pyrochlores — •J. Gronemann[1,2], T. Gottschall[1], C. Salazar[1], J. Hornung[1], T. Herrmannsdörfer[1], A. Islam[3], V. Anand[3], B. Lake[3,4], H. Kaneko[5], H. Suzuki[6], and J. Wosnitza[1,2] — [1]HLD-EMFL, HZDR, Dresden, Germany — [2]Inst. f. Festkörper- und Materialphysik, TU Dresden, Germany — [3]Helmholtz-Zentrum Berlin, Germany — [4]Inst. f. Festkörperphysik, TU Berlin, Germany — [5]Dep. of Quantum Matter, Hiroshima Univ., Japan — [6]Dep. of Physics, Kanazawa Univ., Japan

We have investigated selected pyrochlore compounds in order to study possible nuclear magnetic contributions to the formation of their magnetic ground states and unconventional excitations. For that we focused on $Ho_2Ti_2O_7$ and $Pr_2Hf_2O_7$. Both are representatives for the occurence of spin-ice behavior.[165]Ho and [141]Pr are isotopically pure elements and have large hyperfine enhanced nuclear magnetic moments. The non-spherical [165]Ho nuclei, in addition, carry large electric quadrupole moments. For this reason, these two pyrochlore compounds are well suited to determine possible nuclear magnetic influence. Our specific heat and ac susceptibility data measured at 0.06 K to 10 K suggest a formation of a complex $\vec{F} = \vec{J}+\vec{I}$ coupled ground state which is further modified by electrical field gradients. The ground state F multiplets of $Ho_2Ti_2O_7$ and $Pr_2Hf_2O_7$, in consequence, are accompanied by a total entropy which is significantly larger than the one of a purely electronic CEF ground state doublet and in particular larger than the Pauling residual entropy.

TT 46.9 Wed 15:00 P2/2OG

ESR investigations of disorder effects in organic spin-liquid compounds — •Björn Miksch[1], John A. Schlueter[2], Martin Dressel[1], and Marc Scheffler[1] — [1]1. Physikalisches Institut, Universität Stuttgart, Germany — [2]Material Science Division, Argonne National Laboratory, Argonne, Illinois 60439-4831 and National Science Foundation, Alexandria, Virginia 2223, USA

Although many low temperature properties of the organic spin-liquid candidate κ-$(ET)_2Cu_2(CN)_3$ have been studied experimentally, a comprehensive description is still difficult. Disorder effects have been recently suggested to provide an explanation for the intriguing magnetic and thermodynamic properties. In this study we present electron spin resonance measurements performed with conventional spectrometers as well as with our on-chip approach. This allows us to cover temperatures from 300 K to the mK regime in a broad range of magnetic fields. The results indicate the presence of local moments at very low temperatures supporting the importance of disorder for the low temperature magnetic state.

TT 46.10 Wed 15:00 P2/2OG

Thermodynamic investigations of the quantum-spin-liquid candidate $Ca_{10}Cr_7O_{28}$ — •Ulrich Tutsch[1], Christian Thurn[1], Christian Balz[2,3,4], Bella Lake[3,4], and Michael Lang[1] — [1]Physikalisches Institut, Goethe-Universität Frankfurt am Main, Germany — [2]Neutron Scattering Division, Oak Ridge National Laboratory, Tennessee, USA — [3]Helmholtz-Zentrum für Materialien und Energie, Berlin, Germany — [4]Institut für Festkörperphysik, Technische Universität Berlin, Germany

A quantum-spin-liquid (QSL) is characterized by a coherent and highly entangled ground state without any long-range spin order. One strategy for the realization of such a state is the use of geometrical frustration, as, e.g., encountered in $Ca_{10}Cr_7O_{28}$ with its distorted spin-1/2 kagome bilayer structure. Previous studies have failed to detect any sign of long-range magnetic order in this compound down to 19 mK, its spins staying entirely dynamic. Here, we present low-temperature (40 mK$\leq T \leq$1.7 K) data of the specific heat C and the thermal expansion α for $Ca_{10}Cr_7O_{28}$ at various magnetic fields B up to 12 T [1]. No indications for a phase transition are observed. Instead, a kink-like structure is revealed around 0.5 K, resembling a crossover rather than a phase transition. Both quantities, $C(T)$ and $\alpha(T)$, are significantly affected by already small magnetic fields (<1 T) although a field of about 12 T is needed to open a gap in the magnetic excitation spectrum. These experimental findings support the quantum-spin-liquid hypothesis for $Ca_{10}Cr_7O_{28}$ and promise interesting physics.

[1] J. Sonnenschein *et al.*, Phys. Rev. B **100**, 174428 (2019)

TT 46.11 Wed 15:00 P2/2OG

Nonlocal correlations in the metallic phase of the Kagome Hubbard model — •Josef Kaufmann[1,4], Klaus Steiner[1,2], Andrej Lehmann[3], Daniel Hirschmeier[3], Alexander Lichtenstein[3], Richard Scalettar[2], Karsten Held[1], and Oleg Janson[4,1] — [1]TU Wien — [2]UC Davis — [3]Universität Hamburg — [4]IFW Dresden

In recent years the geometrically frustrated Kagome lattice has been in the focus of many model studies. However, most of them were done in the context of the Heisenberg model, whose ground state is believed to be a spin-liquid. Much less is known about the parent Hubbard model, which includes both electron hopping and local Coulomb repulsion on equal footing. Therefore it is very difficult obtain even approximate solutions.

A very successful approximation is made in the dynamical mean-field theory, where one obtains an auxiliary impurity model. To overcome its inherent restriction to local correlations, we employ the dynamical vertex approximation [1], the dual fermion approach [2], and determinant quantum Monte Carlo [3].

As a result, we obtain sizable non-local components in the self-energy. The effect of geometrical frustration becomes manifest in the magnetic structure factor, which is essentially independent of temperature at low temperatures.

[1] A. Toschi et al., PRB 75, 045118 (2007)
[2] A. N. Rubtsov et al., PRB 79, 045133 (2009)
[3] S. R. White et al., PRB 40, 506 (1989)

TT 46.12 Wed 15:00 P2/2OG

Frustrated quantum magnetism in the Kondo lattice on the zig-zag ladder — •Cassian Plorin, Lena-Marie Woelk, Matthias Peschke, and Michael Potthoff — I. Institut für Theoretische Physik, Fachbereich Physik, Universität Hamburg

We study the phase diagram of the one-dimensional Kondo lattice model with nearest-neighbor hopping t_1 and next-nearest-neighbor hopping t_2 at half-filling using matrix-product-states techniques. Of particular interest is the interplay between geometric frustration, antiferromagnetic ordering of the localized spins, and the Kondo effect.

It is shown that t_2 can induce various magnetic phases such as spin dimerization, quasi-long-range spin-spiral order and short-range incommensurate spin-spiral order – strongly depending on the Kondo exchange coupling J_K. In the strong-J_K regime, the appearance of short-range magnetic order can be explained by perturbative techniques.

The same model but with classical localized spins is investigated as well. Here, we find a qualitatively similar ground-state phase diagram.

In addition we discuss the spin-only Kondo-necklace model on the

zig-zag ladder, which can be seen as an effective theory of the correlated Kondo lattice in the $U \to \infty$ limit. Here, the intriguing question is how the critical point of the J_1-J_2 spin chain affects the phase diagram and whether or not this is linked to the $U = 0$ Kondo lattice.

TT 46.13 Wed 15:00 P2/2OG

The repulsive interactions of the elastic quantum strings. — •Xue-Feng Zhang — Department of Physics, Chongqing University, Chongqing, 401331, China

The elastic quantum string is the quantum topological defects exist not only in the high-Tc superconductivity [1], but also in the frustrated system, such as the hard-core boson on the Kagome lattice [2,3], anisotropic triangular lattice [4] and spin half Ising model with long range interaction in the transverse magnetic field [5]. In this work, we study the repulsive interaction between effective closed strings defined on the bonds of the titled square lattice. By using the large-scale high accuracy exact diagonalization (ED) (error less than 10^{-28}), we find the effective repulsive interactions between the strings are approximately exponential decaying with form $V(r) \approx \exp(-kr^2)$, where r is the distance between strings.

[1] B-X Zheng, et. al, Science **358**, 1155 (2017)
[2] X.-F. Zhang, and S. Eggert, Phys. Rev. Lett. **111**, 147201 (2013)
[3] X.-F. Zhang, Y.-C. He, S. Eggert, R. Moessner, and F. Pollmann Phys. Rev. Lett. **120**, 115702 (2018)
[4] X.-F. Zhang, S.-J. Hu, A. Pelster and S. Eggert Phys. Rev. Lett. **117**, 193201 (2016)
[5] Z. Zhou, Z. Yan, D.-X. Liu, Y. Chen and X.-F. Zhang ongoing work

TT 46.14 Wed 15:00 P2/2OG

Improved EPR spectroscopy on single molecular magnets — •Michael Schulze[1], Daniel Schroller[1], Gheorghe Taran[1], Eufemio Pineda[2], Mario Ruben[2], Christoph Sürgers[1], and Wolfgang Wernsdorfer[1] — [1]Physikalisches Institut, KIT, Karlsruhe — [2]Institut für Nanotechnologie, KIT, Karlsruhe

The quantum nature and large magnetic anisotropies in lanthanide-based single molecular magnets (SMMs) provides potential for interesting applications in quantum computing and information storage. The development of the micro-SQUID technique provides a tool for high-resolution magnetization measurements of SMM single crystals from the mK-range up to several Kelvin. EPR spectroscopy, where different spin states are excited by resonant absorption of radio frequency radiation, serves as a powerful extension of the micro-SQUID technique to gain further insight into the magnetic properties of SMMs. This project strives to improve various features of this combined setup, such as higher coupling strenghts, better thermalization, and coherent spin manipulation of SMMs.

TT 46.15 Wed 15:00 P2/2OG

Electrical read out of the nuclear spin in Tb_2Pc_3 triple decker — •Luca Kosche[1,2], Philipp Schneider[2], Christoph Sürgers[2], Franck Balestro[3], and Wolfgang Wernsdorfer[1,2,3] — [1]Institut für Nanotechnologie, KIT, Germany — [2]Physikalisches Institut, KIT, Germany — [3]Institut Néel, CNRS Grenoble, France

Single-molecular magnets (SMMs) have emerged as an excellent link between the two disciplines of spintronics and molecular electronics. Their ultimate small size, excellent single spin characteristics, and long coherence times at low temperatures make them promising candidates for fundamental quantum operations. In this project we investigate three terminal transistors comprising a SMM trapped in a nanometer sized gap coupled to a back gate thereby forming a quantum dot. The gap is achieved by electromigration of a gold junction fabricated by shadow evaporation. Recent low-noise electrical transport measurements enable the read out of the four nuclear spin states of a single terbium ion in a $TbPc_2$ double decker [1]. Here we pursue to investigate more complex multi-state systems such as the Tb_2Pc_3 triple decker to investigate the interactions between the two terbium nuclear spins.

[1] C. Godfrin et al. ACS Nano 11, 3984 (2017)

TT 46.16 Wed 15:00 P2/2OG

Mean-field study of the magnetocaloric effect in a quasi-one-dimensional bimetallic compound — •Maheshwor Tiwari and Andreas Honecker — Laboratoire de Physique Théorique et Modélisation, CNRS (UMR 8089), Université de Cergy-Pontoise, France

Understanding the nature of all possible ground states, in particular, field-induced phases of antiferromagnets, represents an important first step towards understanding their thermodynamic properties, and in particular the magnetocaloric effect. $MnNi(NO_2)_4(en)_2$, en = ethylenediamine, contains ferromagnetically coupled chains with alternating spins of magnitude 1 and 5/2. Here a self-consistent mean-field calculation of the corresponding mixed-spin model with antiferromagnetic exchange between the chains, single ion anisotropy (D), and Zeeman coupling to a magnetic field parallel to the easy axis gives rise to an antiferromagnetic state and a spin-flop transition. We construct the full phase diagram in the H-T plane and discuss the different magnetic states. The antiferromagnetic interchain coupling gives rise to a low ordering temperature and a low saturation field that promise interesting magnetocaloric properties, as we verify by computation of the thermodynamic properties of the model in a magnetic field.

TT 46.17 Wed 15:00 P2/2OG

Quantum magnetism in copper sulfates and selenates — Maria Rosner[1], Marcus Schmidt[2], Yurii Prots[2], •Helge Rosner[2], Dijana Milosavljevic[2], and Andreas Leithe-Jasper[2] — [1]Cambridge University, Homerton College, Hills Road CB2 8PH Cambridge — [2]Max-Planck-Institut für Chemische Physik fester Stoffe, 01187 Dresden, Germany

Copper sulfates and selenates, quantum magnets exhibiting magnetic spin 1/2 copper sites, show a large variety of crystal structures depending on the amount of crystal water, ranging from water free compounds to up to five water molecules per Cu spin. The different amount of crystal water has a surprisingly strong influence on the magnetic properties of the different species. Here, we present a detailed study of the structure property relation for this compound family based on microscopic grounds.

TT 46.18 Wed 15:00 P2/2OG

Field Control of Magnonic Heat Flow — •Benjamin Köhler and Wolfram Brenig — Institute for Theoretical Physics, Technical University Braunschweig, Germany

Insulating quantum magnets allow for genuine spin transport phenomena without carrier dynamics. Controlling such transport by means of external fields is vital for potential device design. Here we study the thermal conductivity of a two-dimensional square lattice spin-1/2 Heisenberg antiferromagnet in the presence of a homogeneous magnetic and a spatially confined electric field. The former alters the Zeeman energy and the latter the Dzyaloshinskii-Moriya interaction. Both affect the spin-canting which controls the heat flow.

For the magnetic field, we use non-linear spin wave theory and a Kubo approach to evaluate the thermal conductivity taking into account current relaxation via intrinsic magnon decay for finite fields and temperature. We use a real-space approach to spin wave theory for the spatially confined electric field. Results for the heat conductivity as a function of the temperature, the strength of the external field, and shape of the electric-field gated region are presented. Semi-quantitative estimates for attainable variations of the heat conductivity in the context of spincaloric applications are included.

TT 46.19 Wed 15:00 P2/2OG

Temperature evolution of molecular-reorientation modes in CuPOF — •D. Opherden[1,2], C. P. Landee[3], F. Bärtl[1,2], R. Stern[4], I. Heinmaa[4], J. Wosnitza[1,2], and H. Kühne[1] — [1]Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden, Germany — [2]Institut für Festkörper- und Materialphysik, TU Dresden, Germany — [3]Department of Physics, Clark University, Worcester, Massachusetts, USA — [4]Institute of Chemical Physics and Biophysics, Tallinn, Estonia

We present a detailed ^{31}P-NMR spectroscopy and relaxometry study of molecular rotations in the metal-organic compound $[Cu(pz)_2(2\text{-}OHpy)_2](PF_6)_2$ (CuPOF). Here, a freezing of the PF_6 rotation modes is revealed by a step-like increase of the temperature-dependent linewidth, accompanied by broad maxima of the longitudinal and transverse nuclear spin relaxation rates. An analysis based on the Bloembergen, Purcell, and Pound theory quantifies the related activation energies E_a/k_B as 250 and 1400 K. The according characteristic correlation times of the local-field fluctuations, caused by the molecular rotation, are $\tau_0 = 20$ and 3 ps. Further, the second and fourth spectral moment of the ^{31}P absorption line were calculated for a rigid lattice, as well as for different types of PF_6 molecular-reorientation modes. The very good agreement between the experimental angular dependences of the second spectral moment and our numerical calculations clarifies the relevant symmetry axes of the PF_6 rotation modes in the different temperature regimes.

TT 46.20 Wed 15:00 P2/2OG

Low Energy Spin Excitations of $LiFePO_4$ — •Johannes Werner[1], Christoph Neef[1], Sergei Zvyagin[2], Alexey Ponomaryov[2], and Rüdiger Klingeler[1] — [1]Kirchhoff Institute for Physics, Heidelberg University, Heidelberg, Germany — [2]High Magnetic Field Laboratory, Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Spin excitations in single crystalline antiferromagnetic $LiFePO_4$ have been investigated by high-frequency electron spin resonance studies in static and pulsed fields up to 50 T. Several resonance branches are observed, which can be associated with the antiferromagnetic resonance (AFMR) modes as well as with single-ion-like excitations of iron ions at the lithium position (i.e., antisite disorder). Pulsed-field ESR experiments in magnetic fields parallel to the easy *b*-axis clearly show closing of the AFM gap at the spin-reorientation transition at 32 T, previously observed by pulsed magnetisation measurements [1]. The pronounced curvature of the AFM resonance mode cannot be explained in a conventional two-sublattice mean field model. In addition to the AFMR branches, a less intense linear resonance branch is observed in pulsed fields. Its extrapolated zero field splitting fits well to an excitation which a recent neutron study [2] associates to a single-ion-like transition between excited (i.e., non-ground state) CF-split states. Our data however exclude this scenario but we attribute it to the presence of antisite disorder.

[1] J. Werner et al. PRB 99.21: 214432 (2019)
[2] Y. Yiu et al PRB 95.10: 104409 (2017)

TT 46.21 Wed 15:00 P2/2OG

Angular dependence of the Raman scattering intensity of optical phonons in rare-earth germanate pyrochlore single crystals — •Christian Röder[1,2], Nathan Leubner[2], Mathis Antlauf[3], Takashi Taniguchi[4], Marcus Schwarz[3], Edwin Kroke[3], and Jens Kortus[2] — [1]TU Bergakademie Freiberg, Institute of Applied Physics, D-09599 Freiberg, Germany — [2]TU Bergakademie Freiberg, Institute of Theoretical Physics, D-09599 Freiberg, Germany — [3]TU Bergakademie Freiberg, Institute of Inorganic Chemistry, D-09599 Freiberg, Germany — [4]National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki, 305-0044 Japan.

Rare-earth (RE) pyrochlores are one of the most interesting groups of materials to study geometrically frustrated magnetism. In this work, the vibrational properties of RE germanates (RE = Er, Ho, Dy, Tb) of pyrochlore structure were studied by Raman scattering at room temperature. The phonon assignment in the case of similar pyrochlores such as titanates, zirconates or stannates is still debated in literature. Angular dependent Raman measurements were performed in backscattering geometry using single crystals of $Ho_2Ge_2O_7$ and $Dy_2Ge_2O_7$. The observed Raman scattering intensity as function of the azimuthal angle reveals a unique behavior for each phonon mode symmetry. The experimental results are complemented by theoretical simulations of the Raman scattering intensity allowing for an unambiguous assignment of the phonon mode symmetry.

This work was financially supported by German Research Foundation within SFB 1143.

TT 46.22 Wed 15:00 P2/2OG

Combined experimental and theoretical study of $Pr_{0.5}Sr_{0.5}MnO_3$ thin films under tensile strain — •Lokamani Lokamani[1,2], Changan Wang[1], Matthias Zschornak[1,4], Ulrich Kentsch[1], Peter Zahn[1], Bangmin Zhang[3], Shengqiang Zhou[1], and Sibylle Gemming[1,4] — [1]Institute of Ion Beam Physics and Materials Research, HZDR, Germany — [2]Department of Information Services and Computing, HZDR, Germany — [3]Department of Materials Science and Engineering, National University of Singapore, Singapore — [4]Institute of Physics, TU Chemnitz, Germany

Perovskites manganites with the general chemical formula $A_{1-x}B_xMnO_3$ are known to exhibit interesting electronic and magnetic properties, which can be further modified by varying the in-plane and out-of-plane lattice parameters. In this poster, we report a transition from insulator to metal in $Pr_{0.5}Sr_{0.5}MnO_3$ epitaxial thin films by using He ion irradiation. With increasing fluence, the out-of-plane (c-axis) lattice constant expands continuously by defect creation. Although the defect density tends to increase the resistivity, irradiated films show metallic behaviour at low temperature. We also present a comparison using density functional theory including Hubbard-U corrections to account for strongly localized Mn d- and Pr f-electrons.